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In the past three years of this project, we have performed large-scale (10-10 atoms) molecular dynamics (MD) simulations to investigate:

- Structure and mechanical properties of nanostructured ceramics;
- Dynamic fracture in ceramics and nanocomposites;
- Dynamics of oxidation of metallic nanoparticles;
- Simulation of internal stresses at silicon/silicon nitride interfaces;
- Nanindentation of silicon nitride.

These MD simulations have been executed with highly efficient, portable and scalable, multiresolution algorithms including the fast multipole method for the long-range Coulomb interaction, a dynamic load-balancing scheme for mapping irregular applications on parallel machines, and fractal-based data compression for scalable I/O and data communicatns

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CONCURRENT COMPUTING LABORATORY FOR MATERIALS SIMULATIONS

FINAL TECHNICAL REPORT (1997-2000)
AFOSR GRANT NUMBER: F9620-98-1-0086

PROGRAM MANAGER: DR. MICHAEL R. BERMAN

ATOMIC SIMULATIONS OF METAL/CERAMIC INTERFACES, NANOPHASE COMPOSITES, AND MEMS ON PARALLEL COMPUTERS

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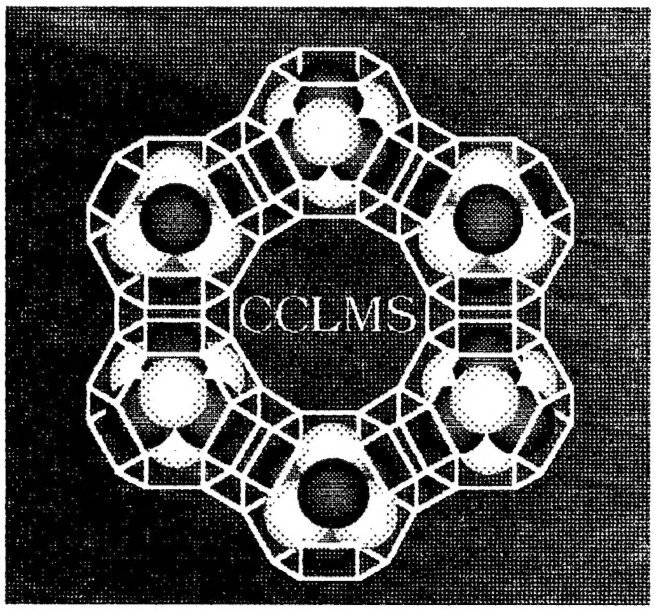

DEPARTMENT OF PHYSICS AND ASTRONOMY
AND
DEPARTMENT OF COMPUTER SCIENCE
LOUISIANA STATE UNIVERSITY

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FINAL PROGRESS REPORT (1997-2000)

ATOMISTIC SIMULATIONS OF METAL/CERAMIC INTERFACES, NANOPHASE COMPOSITES, AND MEMS ON PARALLEL COMPUTERS

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§1 STATUS OF EFFORT

In the past three years of this project, we have performed large-scale (10^6-10^8 atoms) molecular-dynamics (MD) simulations to investigate:

- Structure and mechanical properties of nanostructured ceramics;
- Dynamic fracture in ceramics and nanocomposites;
- Dynamics of oxidation of metallic nanoparticles;
- Simulation of internal stresses at silicon/silicon nitride interfaces;
- Nanoindentation of silicon nitride.

These MD simulations have been executed with highly efficient, portable and scalable, multiresolution algorithms including the fast multipole method for the long-range Coulomb interaction, a dynamic load-balancing scheme for mapping irregular applications on parallel machines, and fractal-based data compression for scalable I/O and data communication. *These research activities have resulted in 48 publications and 76 invited presentations.*[*]

[*] One of our simulations was featured on the cover of *Chemical and Engineering News*.

§2 RESEARCH ACCOMPLISHMENTS

§2.1 STRUCTURE AND MECHANICAL PROPERTIES OF NANOSTRUCTURED CERAMICS

Advanced structural ceramics are highly desirable materials for DoD applications in extreme operating conditions. Light weight, elevated melting temperatures, high strengths, and wear and corrosion resistance make them very attractive for high-temperature and high-stress applications. The only serious drawback of ceramics is that they are brittle at low to moderately high temperatures.

In recent years, a great deal of progress has been made in the synthesis of ceramics that are much more ductile than conventional coarse-grained materials. These so called nanostructured materials are fabricated by *in-situ* consolidation of nanometer size clusters. Despite a great deal of research, many perplexing questions concerning nanostructured ceramics remain unanswered. Experiments have yet to provide information regarding the morphology of pores or the structure and dynamics of atoms in nanostructured ceramics. As far as modeling is concerned, only a few atomistic simulations of nanostructured materials have been reported thus far. This is due to the fact that these simulations are highly compute-intensive: A realistic MD simulation of a nanostructured solid requires 10^5-10^6 time steps and $\sim 10^6$ atoms (each nanocluster itself consists of 10^3-10^4 atoms).

We have performed large-scale MD simulations to investigate the structure and mechanical behavior of nanostructured SiC and SiO_2. Interatomic potentials in these simulations consist of steric repulsion, screened Coulomb potentials due to charge transfer between atoms, charge-dipole interactions to take into account the large electronic polarizability of anions, and three-body bond-bending and bond-stretching terms to include covalent effects. These interatomic interactions are validated by comparing the MD results with: i) measurements of bond lengths and bond-angle distributions in crystalline systems; ii) neutron scattering measurements of positions and relative heights of various peaks in the static structure factor for amorphous SiC and SiO_2; iii) inelastic neutron scattering experiments for phonon densities-of-states of crystalline and amorphous systems; and iv) elastic moduli of crystalline and amorphous systems. In all cases, the MD results are in good agreement with experiments.

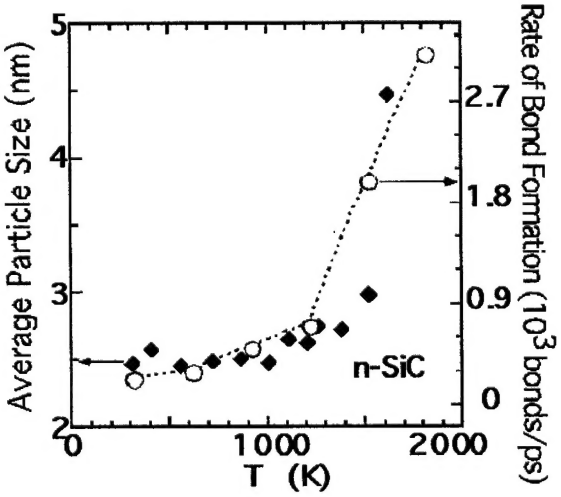

Fig. 1: The onset of sintering is indicated by an increase in the average particle size in the neutron data (◆) and the increase in the rate of bond formation between nanoparticles in the MD results (o). The dotted line is a guide to the eye for the MD results.

Figure 1 shows the results of the first joint experimental and MD study of sintering of nanostructured SiC (n-SiC). In both experiment (solid diamonds in Fig. 1) and simulation (open circles in Fig. 1), the onset of sintering is around 1,500K. The MD simulations provide a microscopic picture of how the morphology of micropores in n-SiC changes with densification. The fractal dimension and the surface roughness exponent of micropores are found to be 2.4 and 0.45, respectively, over the entire pressure range between 0 and 15 GPa. Small-angle neutron scattering at low wavevectors yields a fractal dimension of 2 for pores in n-SiC. MD calculations of pair-distribution functions and bond-angle distributions reveal that interfacial regions between nanoparticles are highly disordered with nearly the same number of 3-fold and 4-fold coordinated Si atoms. The effect of consolidation on mechanical properties is also investigated with the MD approach. The results show a power-law dependence of elastic moduli on the density with an exponent of 3.4 ± 0.1.

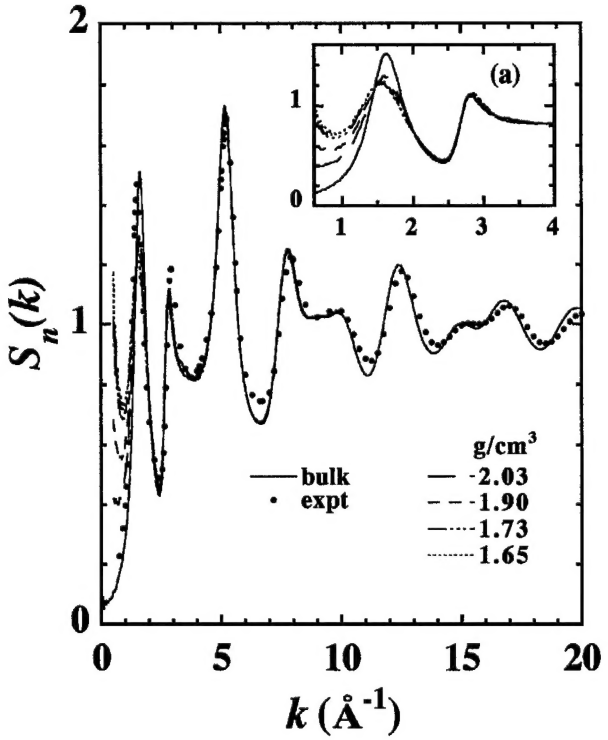

Fig. 2: Neutron-scattering static structure factor, $S_n(k)$, for bulk and nanostructured a-SiO_2. Solid and dashed lines - MD results; solid dots - neutron diffraction results [P. A. V. Johnson *et al.*, J. of Non-Cryst. Solids **58**, 109 (1983)]. Inset (a): magnification of the region around the first sharp diffraction peak.

The simulation of nanostructured SiO_2 involves amorphous nanoclusters, which are obtained from bulk amorphous SiO_2. By sintering at different pressures, we generated nanostructured solids with densities ranging from 76% to 93% of the bulk amorphous density (2.2 g/cm^3). In these solids the morphology of micropores, mechanical behavior, and the effect of nanoscale structures on the short-range and intermediate-range order (SRO and IRO) are investigated. Pores in nanostructured a-SiO_2 are found to have a self-similar structure with a fractal dimension close to 2; the pore surface width scales with the volume as, $W \sim \sqrt{V}$. The MD simulations also reveal that the SRO in nanostructured silica glass is very similar to that in the bulk glass: both of them consist of corner-sharing $Si(O_{1/2})_4$ tetrahedra. However, the IRO in nanostructured silica glass is quite different from that in the bulk glass. In the nanostructured silica glasses the first sharp diffraction peak (FSDP), the signature of IRO, has a much smaller

height and is shifted to smaller wavevectors relative to the FSDP in the bulk silica glass, see Fig. 2. From the partial static structure factors and pair-distribution functions, we find that Si-O and Si-Si correlations in the range of 4-10 Å are primarily responsible for differences in the IRO of bulk and nanostructured silica glasses. We have also investigated the mechanical behavior of nanostructured a-SiO_2. The elastic moduli are found to have a power-law dependence on the density with an exponent of 3.5. These results are in excellent agreement with experimental measurements on high-density silica aerogels.

§2.2 Dynamic Fracture in Ceramics and Nanocomposites

Recently we investigated dynamic fracture in crystalline SiC and GaAs at various temperatures using large-scale MD simulations on 256 nodes of Cray T3E at DoD's Naval Oceanographic Office (NAVO). The simulations were performed with a reliable interatomic interaction scheme that incorporates the ionic and covalent effects in the system. To test the validity of the potentials lattice constants, cohesive energies, elastic moduli, melting temperatures, and phonon densities-of-states of the crystalline systems were calculated. The MD results for these quantities are in good agreement with experimental values.

Dynamic fracture simulations in SiC are performed on a thin-strip sample of 30 million atoms. For this geometry, the mechanical energy release rate, G, of the system can be calculated from the knowledge of the applied strain, ε, and the value of the stress, σ, far ahead of the crack tip: $G = W\sigma\varepsilon/2$. In addition to the mechanical energy release rate, we monitor the crack-tip velocity and local stress distribution at various temperatures. The MD simulations reveal that large shear stresses close to the crack tip cause cleavage fracture at room temperature, see Fig. 3. At elevated temperatures, dissipative effects due to dislocations, micropore formation and coalescence, and crack deflection cause stresses to spread out all over the system, thereby increasing the value of G.

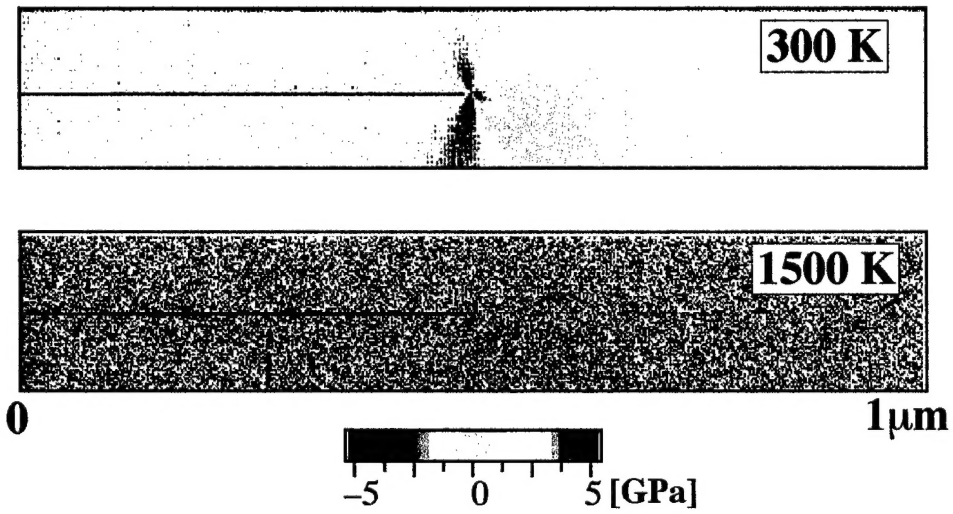

Fig. 3. Shear stress distributions in 30 million atom MD simulations of SiC at 300K and 1500K.

Similar effects are observed in our 100-million atom fracture simulations of GaAs. The MD results also indicate that the brittle-to-ductile transition temperature in GaAs (~ 600K) is close to the experimental value (630-660K). Figure 4 shows snapshots of three different crack fronts in MD simulations of GaAs at room temperature.

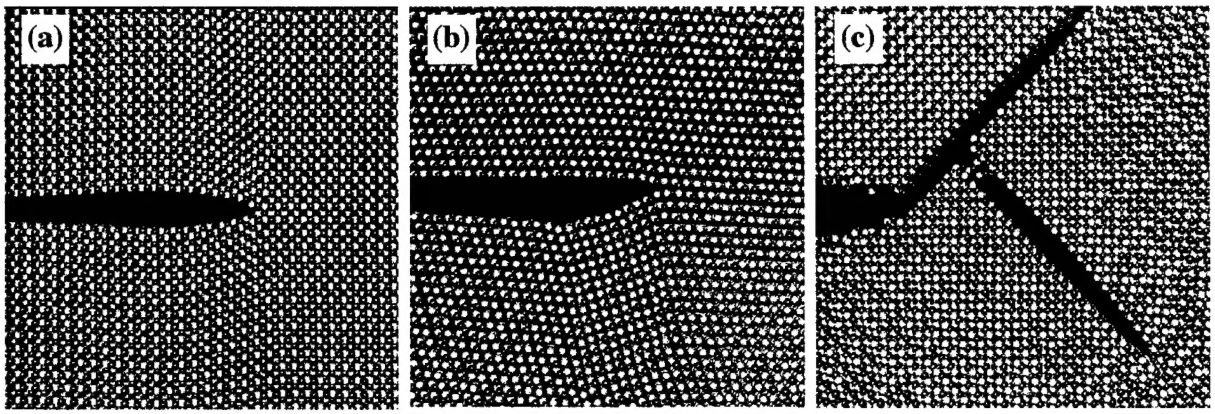

Fig. 4: Snapshots of cracks in MD simulations of GaAs. Crack surfaces are (a) (110), (b) (111), and (c) (001).

One of the most promising materials for high-temperature structural applications is a fiber-reinforced ceramic composite of silicon nitride host (bulk modulus 285 GPa) embedded with fibers of silicon carbide (bulk modulus 220 GPa). The fibers are coated with materials that form weak interfaces between fibers and the matrix. We have performed 10 million atom MD simulations to investigate the effect of interphase structure and residual stresses on fracture toughness in a silicon nitride matrix reinforced by silicon carbide fibers (fiber diameter ~ 3 nm and length ~ 24 nm, see Fig. 5) coated with amorphous silica (bulk modulus 36 GPa) layers of thickness 0.5 nm. Immersive visualization of these simulations reveals a rich diversity of atomistic processes including fiber rupture, frictional pullout, and emission of molecular fragments, which must all be taken into account in the design of tough ceramic composites.

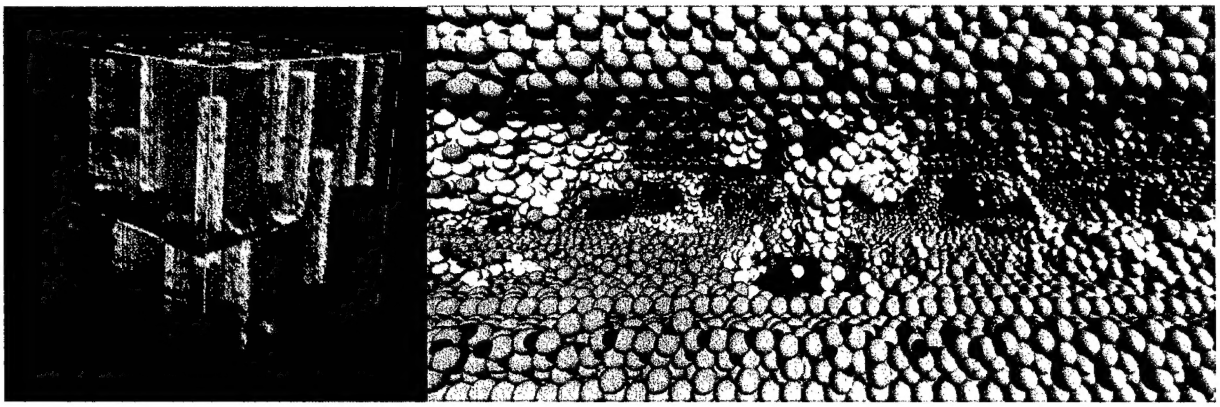

Fig. 5: (Left panel) Fractured silicon nitride (red) ceramic reinforced with silica-coated silicon carbide fibers (yellow). (Right Panel) Close-up of the fractured composite system. Small spheres represent silicon atoms and large spheres represent nitrogen (green), carbon (magenta), and oxygen (cyan) atoms.

§2.3 Dynamics of Oxidation of Aluminum Nanoclusters

In recent years, there has been a great deal of interest in the synthesis of nanostructured composites consisting of metallic nanoclusters coated with a passivation layer. Upon compaction, the passivation layer forms a boundary layer between the isolated metallic grains. The presence of the passivating network is known to have a dramatic effect on the electrical, chemical, and mechanical behavior of the material. In a recent experimental study by Sánchez-López *et al.*, [Nanostruct. Mater. **7**, 813 (1996)] Al/Al-oxide nanocomposites were found to have a metallic shine and an ohmic electrical resistivity that was dependent upon the compaction conditions. The nanocomposite consisted of 300 Å aluminum particles with an interconnected

40 Å oxide layer that prevented the material from falling apart when heated to temperatures above the melting point of aluminum.

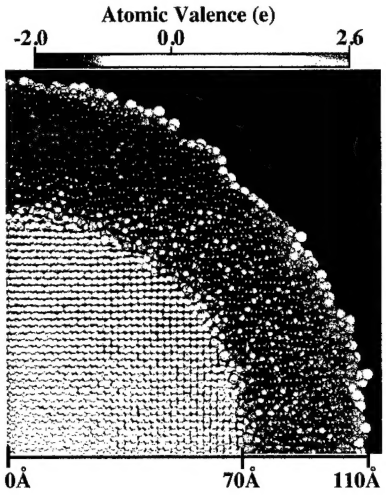

Fig. 6: Snapshot of a small slice (115 Å × 115 Å × 8 Å) of an oxidized Al nanoparticle after 466 ps of simulation time. Larger spheres represent oxygen and smaller spheres represent aluminum; color represents the sign and magnitude of the charge on an atom.

We have performed the first successful MD simulation of oxidation of an Al-nanocluster (diameter 200 Å, see Fig. 6). Structural and dynamic correlations in the oxide region and the evolution of various quantities including surface oxide thickness, diffusivities of atoms, and local stresses have been calculated. The MD simulations are based on a highly reliable interaction scheme developed by Streitz and Mintmire [Phys. Rev. B **50**,11996 (1994)]. It can successfully describe a wide range of physical properties of both metallic and ceramic systems. This scheme is capable of treating bond formation and bond breakage and changes in charge transfer as the atoms move and their local environments are altered. Dynamic charge transfer gives rise to computationally intensive Coulomb interaction which, for the number of atoms necessary in a realistic simulation, requires highly efficient algorithms that map well onto parallel architectures. We use the fast multipole method (FMM) of Greengard and Rokhlin [J. Compute. Phys. **73**, 325 (1987)] for the long-range Coulomb interaction (this reduces the computational complexity from $O(N^2)$ to $O(N)$) with extensions for stress calculations, and the multiple time-step algorithm of Tuckerman *et al.* (J. Chem. Phys. **97**, 1990 (1992), this can further reduce the execution time by an order of magnitude). Both algorithms map well onto parallel architectures.

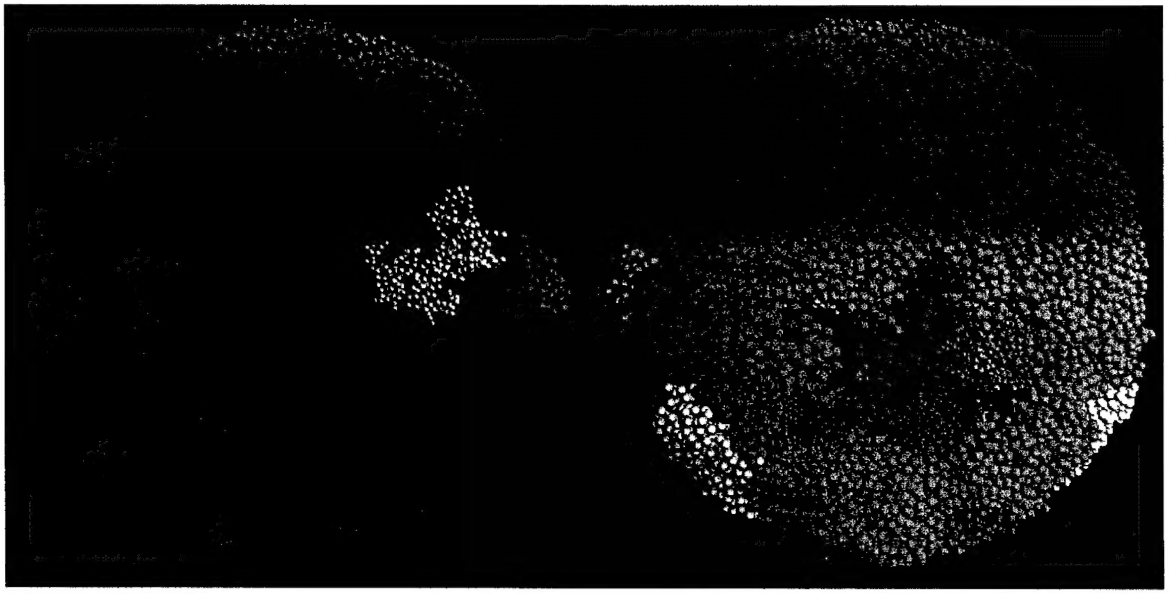

Fig. 7: Initial stage of oxidation of an Al nanoparticle. Size distributions of OAl_4 clusters at 20 ps (left) and 31 ps (right) are shown. Clearly, the clusters coalesce and percolate rapidly.

The MD simulations reveal that an aluminum nanoparticle in an oxygen-rich environment goes through a rapid three-step process culminating in a stable oxide scale in 50 ps.

In the first 5 ps, oxygen molecules dissociate and the oxygen atoms first diffuse into octahedral and subsequently into tetrahedral sites in the nanoparticle. In the next 20 ps, as the oxygen atoms diffuse radially into and the Al atoms diffuse radially out of the nanoparticle, the fraction of six-fold coordinated oxygen atoms drops dramatically. Concurrently, there is a significant increase in the number of O atoms that form isolated clusters of corner-sharing and edge-sharing OAl_4 tetrahedra. Between 30 and 35 ps, clusters of OAl_4 coalesce to form a neutral, percolating tetrahedral network that impedes further intrusion of oxygen atoms into and of Al atoms out of the nanoparticle (see Fig. 7). As a result, a stable oxide scale is formed. Structural analysis reveals a 40 Å thick amorphous oxide scale on the Al nanoparticle. The thickness and structure of the oxide scale are in accordance with experimental results.

§2.4 NANOINDENTATION OF SILICON NITRIDE

Nanoindentation testing is a unique probe of mechanical properties of materials. Typically, an atomic force microscope tip is modified to indent the surface of a very thin film. The resulting damage is used to rank the ability of the material to withstand plastic damage against that of other materials. In addition, a load-displacement curve is constructed from the measured force at each displacement, and the elastic modulus in the direction of the indent can be measured from the initial part of the unloading curve. Commercial nanoindenting apparatus typically has a force resolution of ±75 nN and depth resolution of ±0.1 nm. Recent developments in parallel computing and multiscale algorithms have enabled MD simulations to reach the scale of such commercial nanoindenters, resulting in a better atomic-level understanding of the indentation process.

We have performed 10-million-atom MD simulations of nanoindentation of silicon nitride thin films. Several simulations were performed to determine temperature effects, load-rate effects, and simulation-size effects in crystalline and amorphous silicon nitride. The simulations were run on several different parallel platforms, including the IBM SP's at the U.S. Army Engineer Research and Development Center (ERDC), the Cray T3E at NAVO, and the Origin 2000 at Aeronautical Systems Center (ASC).

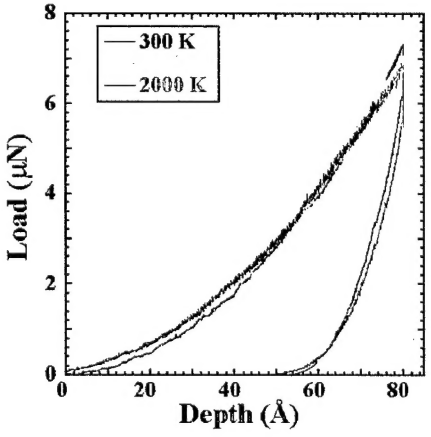

Fig. 8: (left) Load-displacement curves for 300K, 1000K, and 2000K nanoindentation simulations.

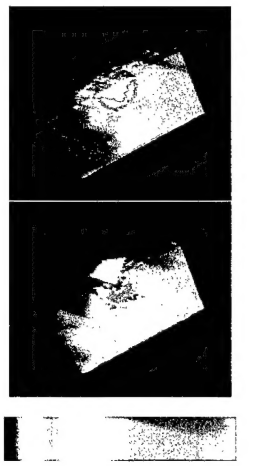

Fig. 9: (right) Local pressure distributions for (top) fully loaded and (bottom) unloaded configurations.

The films had lateral dimensions of 60.6nm x 60.6nm and thickness of 30 nm. Silicon nitride was simulated with an interatomic potential that has been thoroughly validated by comparison with experiment. The films were indented with a square-based pyramidal indenter to

maximum depths of 8-9 nm. Figure 8 shows a comparison of load-displacement curves at three different temperatures. The hardness at 300K (approximately 50 GPa) is reduced to approximately 90% of its value at 2000K. Figure 9 shows the local pressure distribution directly under the indenter for the fully loaded and fully unloaded configurations. These pressure images have been used in conjunction with local bond-angle calculations to characterize a process of local amorphization under the indenter, which is arrested by either piling up of material along the indenter edges or by cracking under the indenter corners.

§2.5 Parallel MD, Dynamic Load Balancing, and Scalable I/O Algorithms

Atomistic simulations discussed in §2.1-§2.4 required considerable computational resources because of long processing times, large system sizes, and compute-intensive interatomic interactions such as long-range Coulomb and three-body covalent forces. Highly efficient, multiresolution algorithms were designed to carry them out on parallel machines. These included algorithms for transferable interatomic potentials involving variable atomic charges and the fast multipole method (FMM).

The multiresolution algorithms are scalable and they have been ported to a number of DoD parallel computers—Cray T3E, SGI Origin 2000, and IBM SP. The parallel efficiency for a 1.02-billion-atom MD simulation of silica is 0.97 and that for a 20.6-million-atom variable-charge MD simulation is 0.96 on 1,024 Cray T3E processors (Fig. 10).

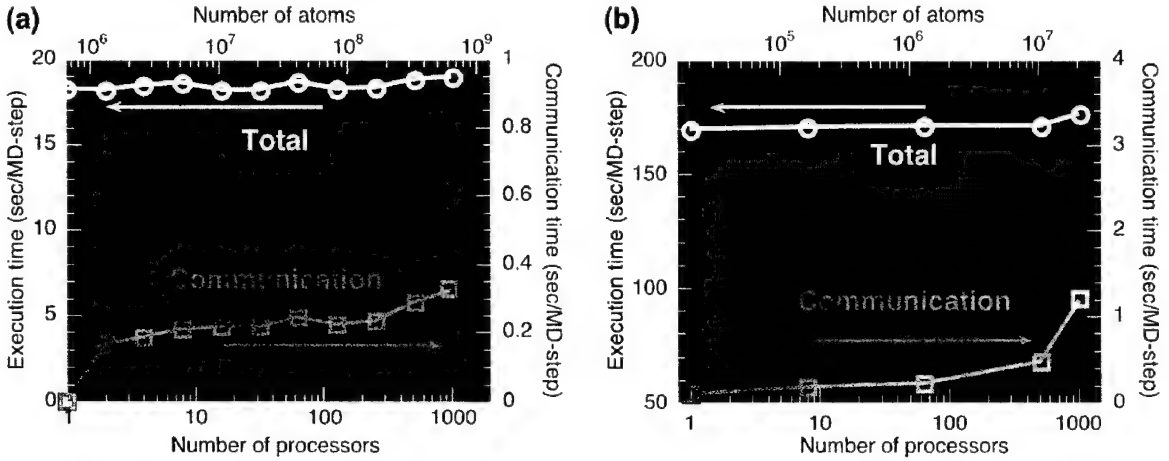

Fig. 10: Scalablity tests of (a) classical and (b) variable-charge MD algorithms on the Cray T3E computer at NAVO. Total execution (circles) and communication (squares) times are plotted for 648,000P atom silica systems for classical MD and 20,160P atom alumina systems for variable-charge MD on P processors (P = 1, ..., 1,024).

We also developed a highly efficient, dynamic load-balancing algorithm for mapping inhomogeneous atomic configurations on parallel machines. The algorithm involves the transformation of atomic cartesian coordinates into curvilinear coordinates using wavelets for a compact representation of abrupt changes in partition boundaries. The workloads for processors were partitioned with a uniform 3-dimensional mesh in the curvilinear coordinate system. The load-imbalance and communication costs were minimized as a functional of the coordinate transformation using the simulated-annealing approach.

We also designed a scalable I/O algorithm for MD simulations. This approach exploits data redundancy to reduce the number of bits stored for each atom. A robust variable-length encoding scheme was used to make the scheme reliable and tolerant to outliers. A flexible interface was provided to the MD code, and significant improvement in the I/O performance was

achieved for actual MD data. The resulting number of bytes per atom does not show any dependence on the number of atoms and it is an order-of-magnitude smaller than that in a conventional I/O scheme.

Finally, we also incorporated a multiple time-scale algorithm in our MD approach. It uses different time steps for long-range and short-range forces. To further speed up simulations, we used a hierarchy of dynamics including rigid-body (or fuzzy-body) motion of atomic clusters.

§3 RELEVANCE TO DoD MISSION

The research we have carried out is related to experimental efforts at DoD laboratories and aerospace industry. Many of these research programs are paced by the status of emerging high temperature materials systems. The DoD Integrated High Performance Turbine Engine Technology initiative and the National Aerospace Plane (NASP) reinforce the need for high-temperature materials in aerospace systems for the twenty-first century. Ceramic composites and coatings represent the most promising technologies for high-temperature applications. Ceramics are widely used to protect materials from heat, wear, oxidation and corrosion, and the Air Force has a thrust to develop ceramic-matrix composites to increase the life of afterburner nozzle components on aircraft turbine engines. The Navy supports the development of thermal-shock-resistant nanocrystalline ceramics and diamond-coated ceramic transparencies. The Army is interested in light-weight ceramics and composites that will increase ballistic protection for armored vehicles. DARPA has a ceramic insertion program to retrofit fielded military systems with state-of-the-art structural ceramics. (Savings of at least $100 million in total life-cycle maintenance costs are expected.) While ceramic coatings enable substantial increases in engine operating temperatures, they remain susceptible to spalling and catastrophic debonding. Computational tools can assist material designers in bringing these material systems to maturity. Improvements in engine efficiency and thrust-to-weight ratio for high performance turbine engines are critical and may play a significant role in determining air superiority. Further progress on NASP is dependent on these new material systems. Metallic nanoparticles have potential applications as energetic materials for advanced propulsion systems. Finally, the computational and visualization tools from this project are useful to those involved in modeling and simulation work in chemical, physical, and biological systems.

§4 TRAINING OF GRADUATE STUDENTS: DUAL-DEGREE PROGRAM

Our graduate students are enrolled in a unique, multidisciplinary program that allows them to obtain a Ph.D. in physics and a MS from the Department of Computer Science. The aim of this program is to provide students with broad-based training in high performance computing and communications (HPCC) and the physical sciences. In connection with this program, we have introduced a number of interdisciplinary courses in the Physics and Computer Science Departments. The Department of Physics has two graduate courses in computational physics that are cross-listed with computer-science courses. The first course deals with multiscale classical and quantum simulations on parallel architectures. The second course, designed for advanced graduate students, covers special topics such as multiresolution algorithms, multigrid methods, wavelets, etc. In the Department of Computer Science, we have introduced three new HPCC courses. Soon two more courses will be added to the computer-science curriculum: (a) Grid computing and (b) immersive and interactive scientific visualization. The courses we have introduced emphasize parallel computing and algorithm design for large-scale scientific

applications. Students have access to a number of parallel machines and an *ImmersaDesk* (see §5) to gain hands-on experience and to perform research on large-scale computational projects.

Our students also have excellent opportunities to broaden their research experience beyond the traditional university based environment. They are involved in our collaborative efforts with computational and experimental scientists at government laboratories, industries, and other universities. These interactions have significantly enhanced the research capabilities of students. Through these contacts, students also have access to excellent parallel computing and visualization facilities at other institutions.

§5 COMPUTATIONAL AND VISUALIZATION FACILITIES

Parallel Computing Facilities

For this research program, several parallel machines were used in our Concurrent Computing Laboratory for Materials Simulations (*CCLMS*). The *CCLMS* consists of two parallel computing laboratories, one in the Department of Physics and Astronomy and the other in the Department of Computer Science. With $3 million in infrastructure enhancement grants from the State of Louisiana, these labs have been equipped with the following parallel machines (see Fig. 11):

- **Digital Alpha cluster**—64 Alpha processors connected via two Gigaswitches and a Fast Ethernet switch;
- **Intel iWarp**—a 64-cell systolic architecture;
- **PC cluster**—166 PCs (550 - 800 MHz Pentium III) linked by a hierarchical network fabric with a Gigabit-Ethernet switch and five Fast-Ethernet switches with gigabit uplinks.

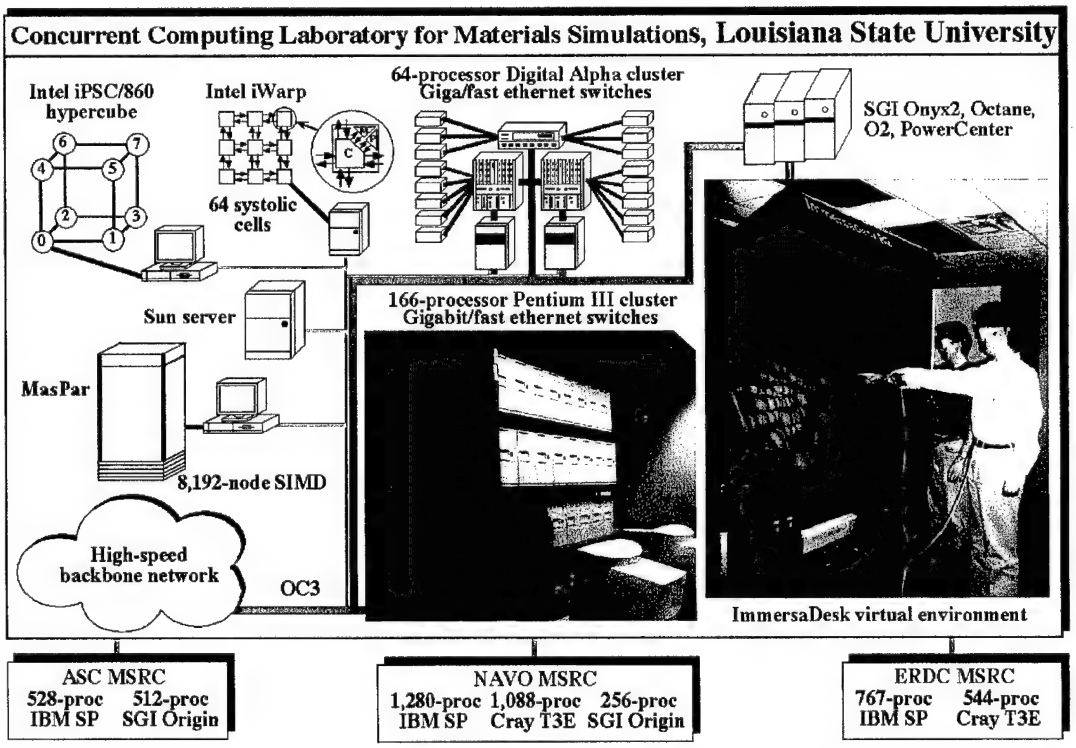

Fig. 11: Computational infrastructure at the *CCLMS*.

In addition, we have received 1.3 million processor-hours of computing per year through the DoD Challenge Application Award to perform large-scale materials simulations on Cray T3E, SGI Origin 2000, and IBM SP computers at DoD's Major Shared Resource Centers.

Virtual Environment Laboratory

We have also established a virtual environment (*VE*) laboratory that features an interactive and immersive *ImmersaDesk* for visualization (see Fig. 12). The VE lab also has a multiprocessor SGI Onyx2/InfiniteReality2, an Octane/MXE, and an 8-processor Power Center graphics servers as well as a number of SGI graphics workstations. Via high-speed networks, the *ImmersaDesk* is fully integrated with the existing parallel machines at the *CCLMS* and with massively parallel computers at national computer centers.

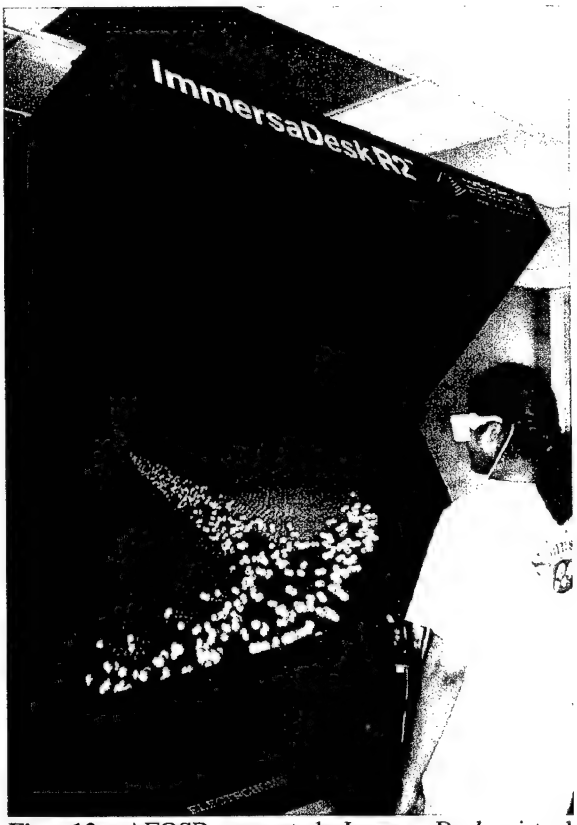

Fig. 12: AFOSR-supported *ImmersaDesk* virtual environment.

§6 PERSONNEL SUPPORTED

Rajiv K. Kalia, Aiichiro Nakano, Priya Vashishta, Timothy Campbell, Hideaki Kikuchi, Sanjay Kodiyalam, Fuyuki Shimojo, and Paulo Branicio were supported by this grant in 1998-99.

§7 PUBLICATIONS

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45. H. Iyetomi, S. Ogata, H. Kikuchi, F. Shimojo, K. Tsuruta, A. Nakano, R. K. Kalia, and P. Vashishta, Material Integration (Kyoto), in press.
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47. E. Lidorikis, M. E. Bachlechner, R. K. Kalia, G. Z. Voyiadjis, A. Nakano, and P. Vashishta, Materials Research Society Symposium Proceedings, accepted for publication.
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§8 INTERACTIONS/TRANSITIONS

A. PARTICIPATION/PRESENTATIONS AT MEETINGS, CONFERENCES, SEMINARS

1. Molecular Dynamics Simulations of Si/Si3N4 Interface and Si/Si/Si3N4 Mesa on Parallel Computers, Symposium on "Theory and Computer Simulation of Materials - Electronic, Structural, and Mechanical Properties", Mexican Materials Research Society, Cancun, Mexico, September 1-4, 1997.
2. Multimillion Atom Simulations of Sintering, Consolidation, and Fracture of High Temperature Materials on Parallel Computers, Workshop on "Computational Materials Physics in the Southeast", Vanderbilt University, Nashville, Tennessee, November 5-8, 1997.
3. Multimillion Atom Simulations of Sintering, Crack Propagation, and Fracture on Parallel Computers, "Noncrystalline Materials", Ohio State University, Columbus, Ohio, November 20, 1997.
4. Multimillion Atom Molecular Dynamics Simulations of Si/Si/Si3N4 Nanopixel-Structural Correlations at Si/Si3N4 Interface, Fracture, and Atomic Level Stresses in the Nanopixel, Workshop on "Interfacialy Controlled Functional Materials: Electrical and Chemical Properties", Schlob Ringberg, Germany, March 8-13, 1998.
5. Large-Scale Molecular Dynamics Simulations of Mechanical Properties of Ultrafine Microstructures on Parallel Computers, Symposium on "Computational and Mathematical Models of Microstructural Evolution", Materials Research Society Meeting, San Francisco, April 13-17, 1998.
6. Multimillion Atom Molecular Dynamics Simulations of Mechanical Properties of Nanostructures in Ceramics and at Semiconductor/Ceramic Interfaces, Symposium on "Computational Modeling of Materials and Processing", American Ceramic Society, Cincinnati, Ohio, May 3-6, 1998.
7 Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers, Fourth Special Symposium on "Advanced Materials", Nagoya, Japan, May 12-14, 1998.

8. Large-Scale Molecular Dynamics Simulations of Amorphous on Parallel Computers, CECAM workshop: "Intermediate Range Order in Network Forming Liquid and Glasses", Lyon, France, May, 18-20 1998.
9. Crack Propagation and Fracture in Nanostructured Ceramics: Multimillion Atom Parallel Molecular Dynamics Simulations, WCTCC 98, Pacific National Northwest Laboratory, Richmond, WA, June 21-23, 1998.
10. Large Scale Simulations of Glasses on Parallel Computers: Nanophase Glasses and Ceramics, The 18th International Congress on Glass, San Francisco, CA, July 5-10, 1998.
11. Large Scale Computer Simulation of Glasses, Workshop on "Modeling Disordered Materials", American Crystallographic Society, Washington DC, July 18-24, 1998.
12. Multimillion Atom simulations of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials, Gordon Conference on "High Temperature Materials, Processing, & Diagnostics", Plymouth, New Hampshire, July 19-24, 1998.
13. Atomic Stresses in Si/Si3N4 Nanopixel - 10 Million Atom Molecular Dynamics Simulation on Parallel Computers, CECAM Workshop on "Surfaces and Interfaces far from Equilibrium", Lyon France, July 27-29, 1998.
14. Atomic Stresses in Si/Si3N4 Nanopixel - 10 Million Atom Molecular Dynamics Simulation on Parallel Computers, "New Developments in High Temperature Ceramics", Istanbul, Turkey, August 12-15, 1998.
15. Multimillion Atom Molecular Dynamics Simulations of High Temperature Ceramics, International Conference on "New Developments in High Temperature Ceramics," Istanbul, Turkey, August 12-15, 1998.
16. Multimillion Atom Simulations of Silica: Crack Propagation and Fracture and Morphology of Fracture Surfaces in Amorphous Silica and Nanophase Silica, SILICA98, Mulhouse, France, September 1-4, 1998.
17. Structure and Dynamic Fracture in Nanophase Silicon Nitride and Silicon Carbide: Multimillion Atom Molecular Dynamics Simulations on Massively Parallel ComputersWorkshop on "Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering," Argonne National Laboratory, Illinois, September 11-12, 1998.
18. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers, "Advanced Materials for Extreme Environments: New Experimental Opportunities in Neutron Scattering", Argonne National Laboratory, Illinois, September 11-12, 1998.
19. Multimillion Atom Simulation of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials, "Computational Studies of Interfacial Phenomena: nanoscale to Mesoscale" Pacific Northwest National Laboratory, Richland, Washington, September 24-25, 1998.
20. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Stresses in Silicon/Silicon/Silicon Nitride Nanopixel, International Union of Materials Research Society, Banglore, India, October 13-16, 1998.
21. Multimillion Atom Simulations of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials and Glasses, Symposium on "Fracture and Ductile vs Brittle Behavior -Theory, Modeling, and Experiments", Materials Research Society, Boston, MA, November 30-December 4, 1998.
22. Multimillion Atom Simulation of Materials on Parallel Computers -Nanopixel and Nanoindentation, "Solid State Physics Symposium 1998", Kurukshetra, India, December 27-31, 1998.
23. Large Scale Atomistic Simulations of Ceramic Materials and Interfaces on Parallel Computers, "Thermo-Mechanical and Electrical Properties of High-Temperature Materials", Maui, January 4-9, 1999.
24. Grand Challenge Materials Simulations: Multimillion Atom Molecular Dynamics Simulations on Parallel Computers, SSI Collaboration Meeting, Jefferson Laboratory, Newport News, Virginia, January 20-22, 1999.
25. Molecular Dynamics Simulations of Materials on Parallel Computers, "Scientific Simulation Initiative", Jefferson Nat'l Laboratory, VA, January 21, 1999.
26. Multimillion Atoms Simulation of High Temperature Ceramic Materials, "The Kick-off Meeting for the Eutectic Research", National Science Foundation, Arlington, VA, February 24, 1999.

27. Massively Parallel Atomistic Simulations of Nanostructured Materials, Physics Department Colloquium, Auburn University, Auburn, Alabama, February 24-25, 1999.
28. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers, Symposium on "Spanning the Size Scales in Materials Phenomena", American Physical Society Centennial Meeting, Atlanta, Georgia, March 22-26, 1999.
29. Crack Propagation and Fracture in Nanophase Materials - Multimillion Atom Molecular Dynamics Simulation on Parallel Computers, "Nanocomposites: Design and Applications", Anchorage, Alaska, March 28-April 2, 1999.
30. Designing Novel Materials on Parallel Computers, Links for Success, The 1999 Annual Board of Regents Louisiana NSF EPSCoR Conference, Pennington Biomedical Research Conference Center, Baton Rouge, Louisiana, April 13-14, 1999.
31. Multimillion Atom Simulations of Crack Propagation, Fracture, and Nanoindentation in Ceramic Materials, "High Strength Steels - Processing and Applications", Ranchi, India, April 14-15, 1999.
32. Large Scale Materials Simulations on Parallel Computers, "Computational Materials Science Network on Ceramic/Polymer Interfaces", Sandia National Laboratory, Albuquerque, NM, April 22-23, 1999.
33. Large Scale Simulations of Glasses on Parallel Computers: Nanophase Glasses and Ceramics, NATO Advanced Study Institute on "Physics of Glasses: Structure and Dynamics", Corsica, France, May 10-22, 1999.
34. Computational Assisted Development of High Temperature Structural Materials, Ninth Annual DoD High Performance Computing Modernization Program Users Group Conference, Monterey, California, June 7-10, 1999.
35. Multimillion Atom Molecular Dynamics Simulations of Ceramic Materials and Interfaces on Parallel Computers, "International Conference on Advanced Materials", Beijing, China, June 13-18, 1999.
36. Multimillion Atom Simulations of Nanostructured Materials on Parallel Computers - Molecular Dynamics Method and Its Applications, "Computational and Applied Mathematics", St. Louis, MO, August 9-11, 1999.
37. Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials on Parallel Machines, ACS Annual Meeting in New Orleans, August 22-26, 1999.
38. Multimillion Atom Molecular Dynamics Simulations of Nanostructured Materials on Parallel Machines, International Materials Research Congress, Symposium: Theory and Computer Simulation of Materials, Cancun, Mexico, August 29 - September 2, 1999.
39. Atomistic Simulations of Nanoindentation of Silicon Nitride on Parallel Computers, "IMRC -Theory and Computer Simulation of Materials ", Cancun, Mexico, August 30-September 3, 1999.
40. Multimillion Atom Simulations of Nanostructured Materials on ParallelComputers - Sintering and Consolidation, Fracture, and Oxidation, "International Conference on Computational Physics ", Kanazawa, Japan, October 11-13, 1999.
41. Atomistic Simulations of Nanostructures: Multimillion Atom Molecular Dynamics Simulations on ParallelComputers, "Foresight Conference on Molecular Nanotechnology ", San Jose, CA, October 15-17, 1999.
42. Massively Parallel Materials Simulations, Colloquium in the Department of Chemical Engineering, Univ. of Cincinnati, October 21, 1999.
43. Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters, CERCA, Montreal, Canada, December 8, 1999.
44. Multiscale Simulations of Nanostructred Materials on Massively Parallel Compters, Steacie Institure for Molecular Sciences, National Research, Council of Canada, Ottowa, Canada, December 10, 1999.
45. Computational Assisted Development of High-Temperature Structural Materials, "Defense Science Board Presentation", Washington, DC, February 4, 2000.
46. Multi-Million Atom Molecular Dynamics Simulations of Metal/Ceramic and Semiconductor/Ceramic Interfaces on Parallel Computers, "Workshop on Process Modeling of Laminated Multilayer Ceramic Systems", Motorola University,Tempe, Arizona, March 1, 2000.
47. Mulltimillion Atom Simulation of Nanostructured Materials on Parallel Computers – Sintering and Consolidation and Fracture and Oxidation, "The Materials Society (TMS)", Nashville, TN, March 12-16, 2000.

48. Parallel Multiscale Simulations of Nanostructured Materials, CSW 2000 EPOCHAL TSUKUBA International Congress Center, March 13-15, 2000.
49. Molecular Simulations of Solids: Metals, Semiconductors, Ceramics, and Glasses, "International Comparative Study of Applications of Molecular and Materials Modeling", Washington, DC, March 14, 2000.
50. Information Technology and the Dual-Degree Program, Amercian Physical Society, Minneapolis, Minnesota, March 20, 2000.
51. Large-Scale Atomistic Simulations of Solid State Materials Modeling Many Millions of Atoms on Parallel Computers, "American Physical Society ", Minneapolis, March 22-24, 2000.
52. Parallel Multiscale Simulations of Nanostructured Materials, Iowa State University and Ames Research Laboratory, Ames, Iowa, April 3, 2000.
53. Multiscale Simulations of Oxidation and Fracture in Nanostructured Solids, HPaC Seminar, TU Delft, The Netherlands, April 14, 2000.
54. Multimillion Atom Simulations of Materials on Parallel Computers - Past, Present and Future, "Celebrating the Success of LSU Computer Science" Baton Rouge, LA, April 14, 2000.
55. Parallel Multiscale Simulations of Nanostructured Materials, MD Meeting, University of Illinois at Urbana, April 16-17, 2000.
56. Multimillion Atom Simulations of Nanophase Materials on Parallel Computers, "Seminars on Humanity 3000- Nanotechnology In the Future", Foundation for the Future, Bellevue, WA, April 21, 2000.
57. Massively Parallel Multiscale Simulations of Nanostructured Materials, Intel Corporation, May 1, 2000.
58. Massively Parallel Multiscale Simulations of Nanostructured Ceramics, American Ceramic Society Symposium on Advances in Theory, Modeling, and Simulations of Materials, St. Louis, Missouri, May 3, 2000.
59. Computer Simulations of Ceramic Interfaces, "AFOSR Meeting on Ceramic Materials and Composites" Saint Louis, MO, May 4-5, 2000.
60. Computer Simulations of Ceramic Interfaces, AFOSR Contractors' Meeting in Ceramic Materials and Composites, St. Louis, Missouri, May 5, 2000.
61. Multimillion Atom Simulations of Materials on Parallel Computers - Past, Present and Future, "XXIII Encontro Nacional de Física da Matéria Condensada", São Lourenço, Minas Gerais, Brasil, May 11-13, 2000.
62. Multi-Million Atom Simulation of Sintering and Consolidation on Parallel Computers, "SIAM Conference on Mathematical Aspects of Materials Science", Philadelphia, PA, May 23, 2000.
63. Recent Research Activities in Material Sciences at LSU: Introduction to Concurrent Computing Laboratory for Materials Simulations (CCLMS), "Niigata University-LSU Symposium", Niigata University, Niigata, Japan, May 30, 2000.
64. Computational Assisted Development of High-Temperature Structural Materials, "DoD High Performance Computing Modernization Program Conference", Albuquerque, NM, June 5-8, 2000.
65. Parallel Molecular Dynamics Simulations of Nanostructured Materials, Corsica Meeting on Fracture, June 15-17, 2000.
66. Large-Scale Atomistic Simulations of Amorphous Polymers and Ceramic/Polymer Interfaces on Parallel Computers, "American CrystallographicSociety ", Minneapolis, MN, July 22-27, 2000.
67. Parallel Molecular Dynamics Simulations of Nanostructured Materials, Canadian Computational Chemistry Meeting, Bishop University, Lennoxville, Quebec, Canada, July 31 - August 3, 2000.
68. Multimillion Atom Simulation of Materials on Parallel Computers -Nanopixel, Interfacial fracture, Nanoindentation, and Oxidation, "MAPINT Symposium on Multidisciplinary Applications and Interoperable Computing", Dayton, Ohio, August 17, 2000.
69. Simulations of Nanostructured Materials, TU Delft, The Netherlands, September 25, 2000.
70. Atomistic Modeling Capabilities for Sintering of Ceramics and Fracture at Interfaces, "NSF Multi-University I/UCRC Ceramic and Composite Materials Center", Piscatway, NJ, September 27-28, 2000.
71. Multimillion Atom Simulation of Nanostructured Materials – Dynamic Fracture, Nanoindentation, and Oxidation, "International Conference on Engineering & Technological Sciences 2000 –

Advanced Materials", Beijing, China, October 10-14, 2000.

72. Large Scale Molecular Dynamics Simulations of Materials on Parallel Computers, "ACAT2000 Conference", Fermilab, IL, October 18-19, 2000.
73. Large Scale Molecular Dynamics Simulations of Nanostructured Materials on Parallel Computers– Dynamic Fracture, Nanoindentation, and Oxidation, "Joint CNRS (France)-NSF (USA) Nanomaterials Workshop – Nanomaterials Toward Engineering Applications", Montreal, Canada, October 20-25, 2000.
74. Multiscale Materials Simulations: Importance of Neutron Scattering, Argonne National Laboratory, November 20, 2000.
75. Multiscale Materials Simulations, National Research Council, Ottawa, Canada, November 23, 2000.
76. Multiscale Simulations of Nanostructured Solids on Massively Parallel Computers, International Conference on Science & Technology of Nanostructured Materials, Puri, India, January 4-8, 2001.

B. CONSULTATIVE AND ADVISORY FUNCTIONS TO GOVERNMENT LABORATORIES AND AGENCIES

- Member of the executive committee of the DOE's National Energy Research Supercomputer User Group (NERSC).
- Served on the advisory committee of a DOE supported workshop on "Probing Advanced Materials for Extreme Environment: New Experimental Opportunities in Neutron Scattering." The workshop was held in connection with the DOE initiative on Spallation Neutron Source to be built at Oak Ridge.
- Editorial board, Journal of Physics: Condensed Matter.
- Associate Editor-in-Chief, Computing in Science and Engineering.
- Serving on World Technology Evaluation Center (WTEC) Panel on Applications of Molecular Modeling.

C. TRANSITIONS

Government Laboratories

- Collaborated with Drs. C. Woodward and D. Dimiduk at the AFRL (Wright Patterson Research Site) on DoD's Challenge project "Computational Assisted Development of High Temperature Structural Materials".
- Collaborated with Dr. S. Rodgers at the AFRL (Edwards) on a project involving the oxidation of metallic nanocluster. A joint paper was published recently in the Physical Review Letters.
- Wrote a MURI proposal with Drs. R. Pachter (AFRL, Wright Patterson), M. Gordon (Iowa State Univ. and Ames Lab), and G. Voth (Univ. of Utah).
- Collaborating with Dr. S. Saini at NASA Ames on algorithm design and implementation of large-scale materials simulations on NASA's Information Power Grid.
- Collaborating with Dr. A. Sayir at NASA Lewis on experimental and simulation studies of hgih-temperature ceramic eutectics.
- Collaborating with Dr. C. Loong at Argonne National Laboratory on a joint neutron scattering and molecular-dynamics study of nanostructured ceramics.

Industry

- Collaborating with Dr. S. Shankar's simulation and modeling group at Intel Corporation on atomistic simulation of electronic devices.
- Collaborating with Dr. David Wilcox's group at Motorola.

Universities

- Collaborating with Dr. A. Madhukar's group at the University of Southern California on a MURI project involving process modeling of devices.

§9 NEW DISCOVERIES, INVENTIONS OR PATENT DISCLOSURES

None.

§10 HONORS AND AWARDS

Rajiv K. Kalia was honored with the 1999 LSU Distinguished Faculty Award and Aiichiro Nakano with the 1999 LSU Alumni Association Faculty Excellence Award.